

1,1-dimethoxyhexan-2-one
6344-10-1 | DTXSID70287285

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -43.2 °C

Global applicability domain: Inside

Local applicability domain index: 6.64e-01

Confidence level: 6.26e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Butoxyethyl acetate</div> <div>Measured: -63.0</div> <div>Predicted: -54.2</div>	<div>Image not found</div> <div>2-Ethoxyethyl acrylate</div> <div>Measured: -47.0</div> <div>Predicted: -54.7</div>	<div>Image not found</div> <div>2-Ethoxyethyl acetate</div> <div>Measured: -61.7</div> <div>Predicted: -56.7</div>
<div>Image not found</div> <div>2-Methoxyethyl acetate</div> <div>Measured: -70.0</div> <div>Predicted: -63.1</div>	<div>Image not found</div> <div>Dimethyl decanedioate</div> <div>Measured: 38.0</div> <div>Predicted: 1.98</div>	